

# **Edward Teller's Scientific Life**

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# **Edward Teller's Scientific Life\***

## **Physics Today**

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Edward Teller was one of the great physicists of the twentieth century. His career began just after the key ideas of the quantum revolution of the 1920's were completed, opening vast areas of physics and chemistry to detailed understanding. Thus, his early work in theoretical physics focused on applying the new quantum theory to the understanding of diverse phenomena. These topics included chemical physics, diamagnetism, and nuclear physics. Later, he made key contributions to statistical mechanics, surface physics, solid state, and plasma physics. In many cases, the ideas in these papers are still rich with important ramifications.

Teller's career was clearly divided between two distinct but overlapping phases. The first, from 1928 to 1952, was devoted to basic science and university life; in the second part, beginning with the discovery of fission in 1939, his chief (but not sole) focus became the application of physics to defense, and the founding (in 1952) and development of the Livermore Lab. This short article, though inevitably incomplete, is an attempt to give a flavor of his scientific achievements. The companion article by Harold Brown and Michael May addresses the second part of his career.

Our appreciation for Teller's approach to physics is based on the authors' bi-weekly conversations with him. One of us, MSW, joined the Physics Department at Livermore in 1968, and began collaborating with Teller at that time. SBL joined the lab in 1986. His collaboration and conversations with Teller began in 1989. In these conversations, the topic of the day might have been a recent discovery or new idea, or perhaps an older subject deserving further analysis. As many would confirm, these interviews were partly a Socratic dialogue and part never ending graduate school general exam. Though initially formidable, the interaction quickly became quite pleasurable. Almost always, Teller was able to put his finger on 'what was going on" in the problem at hand with uncanny clarity. One typically came away with a much deeper understanding – even if one was the supposed expert on the subject at hand. In this age of greater mathematical formality and narrow specialization, it was a rare pleasure to be asked to try to figure out on the spot: "where are the electrons," "what do the wave functions actually look like," "would a semi-classical approximation capture the essence of the problem," and so on.

As was true of the other great Hungarian theoretical scientists born just after 1900 (nicknamed the 'Martians' for their astounding brilliance), Teller's thinking was distinguished by a unusual, innovative blend of abstract inquiry and application. Specifically, Teller, initially directed by his family toward a practical career in chemical engineering, never lost his interest in applied questions, and this interest animated his early focus on the application of quantum mechanics to the microscopic understanding of molecular behaviors. Later, his desire to see practical consequences of basic science influenced his interest in defense matters as well as his later leadership of the Livermore branch of the UC Davis Department of Applied Science, sometimes termed 'Teller Tech.'

Often using dialogue as a path to scientific discovery, Teller commonly asked a crucial question and then found a collaborator to work with him on the solution. This explains his large number of two or multiple author papers. His interests were truly broad, though he was perhaps guilty of not following up after the initial discovery was made. To the end, his spirit of inquiry led him to seek out young people to teach him about current developments in physics.

Teller began his scientific work in 1928 under the direction of Werner Heisenberg at the University of Leipzig. Following the initial work of Walter Heitler, Fritz London, John Van Vleck, E. Bright Wilson, and others applying the new quantum mechanics to molecules, Teller's 1930 thesis addressed the excited states of the most fundamental molecule: the hydrogen molecular ion. Teller always related with relish that during that period he lived in Heisenberg's house and that he was doing the needed numerical calculations at all hours on a noisy mechanical calculator. Heisenberg declared the work complete at the point when he tired of the racket made by the calculator.

Teller's work on the hydrogen molecular ion was the first of a series of significant papers in the 1930's applying quantum mechanics to understanding molecular physics. In this series of papers, with many collaborators, <sup>2</sup> Teller developed the formalism and analyzed the spectral and structural consequences of vibrational – electronic couplings in molecules. The 1937 proposal of the Jahn-Teller theorem<sup>3</sup> was the culmination of this period. This theorem states that nominally symmetrical molecules (except for linear cases) will spontaneously deform so as to break the electronic term quantum mechanical degeneracy thereby producing a unique ground state. Because the theorem covers a fascinating array of soft electron-nuclear coupling phenomena, it is no surprise that it continues to be widely applied to both isolated molecular systems and the solid state. Though it is impossible to give any kind of realistic assessment of the scientific influence of the Jahn-Teller effect in this short space, one might cite the discovery of high temperature superconductivity as a recent example of that influence. J. Georg Bednorz and K. Alex Muller say they were motivated to study various perovskites<sup>4</sup> because these materials exhibit very strong Jahn-Teller distortions offering the promise of large electron couplings (see 1st side bar insert- Jahn-Teller distortion of the Cu-O octahedron).

Another illustration of the continuing significance of Teller's papers during this period concerns a generalization<sup>5</sup> of the well known 1929 result of Eugene Wigner and John

Von Neumann on quantum mechanical level repulsion in the case of a single real Hamiltonian tuning parameter. Teller's generalization to level intersections controlled by two or more real degrees of freedom resulted in a fascinating array of topological possibilities, characterized by a linear dependence on the tuning variables. Later, in the hands of Gerhard Herzberg and H. Christopher Longuet-Higgins,<sup>5</sup> an analysis of the consequences of Teller's result for the global behavior of the wave functions gave the first molecular physics example of Berry's topological phase.

Teller continued to have a close relationship with Heisenberg after leaving Leipzig for Gottingen in 1930. On a return visit to Leipzig, Heisenberg posed to Teller the conundrum offered by Lev Landau's 1930 computation of the diamagnetic susceptibility of a free electron gas.<sup>6</sup> This was in flat contradiction to a classical argument due to Bohr and van Leeuwen that there should be no diamagnetism at all! This is because in a classical computation of the partition function, the influence of an external vector potential can be absorbed into the momentum sum. Teller gave a physical argument explaining why Landau was correct in terms of the population and current of what one would now call the skipping orbit or "edge state."

After the Nazis came to power 1933, conditions for Jews in German universities rapidly deteriorated, and Teller left Germany, first going to the Bohr Institute in Copenhagen, then to University College, London under a grant from the Rockefeller foundation, and finally to the United States. In the United States, Teller was respectively a Professor at George Washington University from 1935 – 1941, and at Columbia University from 1941 until he joined the Manhattan Project in 1943.

Teller met Landau first in Leipzig and then later at the Bohr Institute in Copenhagen where he also met George Gamow. They were two essential influences on Teller's thinking during the 1930's. Teller loved to bounce ideas off Landau, and credited him with stimulating the ideas that became the 'Jahn-Teller' theorem. Together they presented a quantum mechanical description of sound dispersion and attenuation based on the idea of the dephasing of sound modes due to their coupling to internal degrees of freedom of the molecules in the medium. This led to immediate predictions of the damping rate dependence on molecular composition and temperature.

Teller's fruitful collaboration with Gamow at George Washington University began when Teller arrived in the United States in 1935, and included the discovery of the Gamow-Teller transition rules, and several astrophysical papers that include work on red giants and early analyses of thermonuclear reaction rates. As with the Jahn-Teller effect, one cannot attempt a compact assessment of the consequences of the 'nucleon spin flip' Gamow-Teller alternative to the Fermi selection rule. Such a history would necessarily thread through the developing phenomenology of nuclear beta decays and emerge in the 1950's with Lee and Yang's discovery of parity violation and the subsequent proposal of the V-A theory of the weak interaction. The Gamow-Teller paper itself shows and exploits an incisive mastery of the known nuclear decay phenomena of that era. (see GT side bar insert).

Teller's work in nuclear physics also includes his papers with a very young Julian Schwinger laying out the phase shift analysis of low energy neutron interference scattering from hydrogen molecular targets, as well as his striking proposal (many years later in 1948) with Maurice Goldhaber of the explanation of giant photonuclear resonances in nuclei. Motivated by experiments on ( ,n) reactions and photo fission showing evidence for resonances at energies (16 -30 MeV) varying inversely as the sixth root of the nuclear mass , they made the bold proposal that, universal to all nuclei, the protons and neutrons could act as interpenetrating fluids capable of dipole vibration. Their discovery was a key step in defining large collective nuclear oscillations. Charles Critchfield, John Wheeler, and Eugene Wigner were also collaborators on nuclear physics.

Over the decades, Teller's career was often marked by his attraction to puzzling experimental results or theoretical and computational challenges. Frequently, as in the diamagnetism example, his analysis led to resolutions that carried the seeds for new ways of thinking. Examples include the already mentioned Jahn-Teller effect and Gamow-Teller selection rules, and the Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller<sup>11</sup> method in statistical mechanics. The Brunauer-Emmett-Teller equation of state in surface physics, <sup>12</sup> and his work with Breit on the two photon decay of the 2s state of hydrogen, <sup>13</sup> were incisive responses to experimental challenges. In 1947, Teller, with Fermi and Weiskopf, by carefully considering the experimental consequences for particle stopping and subsequent decay, gave the definitive analysis that showed that the muon could not be Yukawa's pi meson<sup>14</sup> (Powell's discovery of the real pion followed in the same year).

In a somewhat different vein, he invented (or co-invented) simple examples and general rules that got to the heart of an important question in quantum mechanics or statistical mechanics. examples include the Poschl-Teller exemplar of anharmonic quantum mechanics, and the Ashkin-Teller generalization of the Ising Model. The latter was motivated directly by two simultaneous requirements. Can one make a simplified model capturing the essential features of the a freezing transition dependent on bond orientation due to differing strengths between atoms and yet still retain the Ising feature of a duality transformation guaranteeing a mapping between the low and high temperature phases? The answer was yes, and the Ashkin-Teller model now takes its place as one of a sequence of exactly soluble two dimensional statistical mechanics models.

On a quite different kind of solid state question, with Lyddane and Sachs, he gave the general rule, with broad applications including ferroelectricity, that the ratio of the transverse to longitudinal phonon frequencies (squared) in crystals is given by the ratio of the dielectric function in the limits of infinite and zero frequency:

$$_{\rm T}^2/_{\rm L}^2 = ()/(0).^{16}$$

As will be noted again later, Teller frequently returned to the Thomas-Fermi picture of the atom and was interested in both its power and limitations. In an insightful paper written for Wigner's 60<sup>th</sup> birthday festschrift, Teller showed the impossibility of

molecular binding in the Thomas-Fermi-Dirac approximation.<sup>17</sup> Later, when Lieb and his collaborators<sup>16</sup> beautifully analyzed the properties of matter under the Thomas-Fermi-Dirac and Thomas-Fermi-von Weizacker approximations to full quantum mechanics, Teller's result played an important role.

In some cases, his insight is connected to a still open question. After the discovery of the Van Allen belts in 1957, and simultaneously stimulated by interest in the mirror machine concept for fusion, Teller and Northrop addressed the idealized "Stormer" problem of the motion of a point charge in a dipole magnetic field. After taking into account the conservation of energy and the z component of the angular momentum, four degrees of freedom remain allowing for the possibility of either chaotic or regular motion. They discovered an additional adiabatic invariant beyond the magnetic moment and longitudinal invariants and conjectured that therefore the problem might be exactly solvable, perhaps giving insight into the stability of the van Allen belts. Subsequently, however, Dragt and Finn showed numerically that the Stormer problem has a homoclinic point and therefore cannot be exactly solvable – still leaving open the role (if any) of Teller and Northrop's approximate invariant in the stability of the Van Allen belts. 18

Teller's interest in the physics underlying applied subjects was particularly strong in the areas of the properties of matter at high energy density. Before either Teller or Hans Bethe had official connections with the Manhattan Project, in 1941 they authored a detailed study of the deviations from thermal equilibrium in shocks under the auspices of the Army Aberdeen Research Laboratories. 19 Even earlier, in 1939, with David Inglis, he had proposed a theory of dense plasma continuum lowering based on the criterion that the Rydberg states merge with the continuum when their Stark splittings due to the neighboring ions causes them to overlap. Later, Teller initiated some of the earliest work during and after the Manhattan project on the equation of state of hot dense matter. These papers include the Feynman-Metropolis-Teller extension of the Thomas-Fermi model of the atom to finite temperature and the numerical methods to approximate such equations of state such as the already mentioned 'Metropolis method.' Furthermore, with Frederick de Hoffman (then at Los Alamos), with whom he also collaborated closely on defense issues, he worked out the analogs of the Rankine-Hugoniot shock equations for relativistic magneto-hydrodynamics. In the 1960's at Livermore, having championed both new models for high temperature equations of state and the application of large scale computing, he, with Brush and Shalin, published the first Monte Carlo analysis of the liquid-solid phase transition of the One Component Plasma. In general in these areas, he usually collaborated with members of the Los Alamos and Livermore labs.<sup>20</sup>

Teller always felt strongly that the advances in 'high energy density physics' being made for applied purposes would correspondingly lead to key developments in basic science. It is likely that this view grew from three sources. The first was his lifelong conviction that the best basic science develops hand and hand with applications. The second was his personal involvement in the both the development of nuclear weapons and his simultaneous desire to discover peaceful applications of nuclear technologies. Finally, his increasing isolation from much of the physics community meant that he only learned second hand about the great developments in other physical regimes, such as particle and

condensed matter physics, from the fifties through the end of the century. Thus Teller was a key motivator of work at Livermore that grew naturally out of the basic defense effort. This included inertial fusion, high power lasers and their applications, applications of x-rays, and high performance computing.

Edward Teller was a great physics teacher and mentor. Colleagues and students still recall his particular personal warmth. Over his long career, he had many students. Here we mention just a few. With Renner, an early student in Gottingen, he began the studies of the symmetry of linear molecules that eventually led to the Jahn-Teller theorem. His paper with Julius Ashkin formed the basis of Ashkin's thesis at Columbia. Also at Columbia, Teller sponsored Arthur Kantrowitz's thesis on the generation of hypersonic molecular beams. Chen Ning Yang's thesis at Chicago was a beautiful generalization of work Teller did with Konopinski on deuteron-deuteron interactions. Marshall Rosenbluth was also Teller's student at Chicago during this period. Though not a student of Teller's, Maria Goeppert Mayer credited him as an important mentor. They collaborated through the 1940's, writing in 1949 one of the early papers attempting to understand the nucleosynthesis of heavy elements. After 1953, Teller was also Professor of Physics at UC Berkeley, where his enormously popular basic physics course (Physics 10) was attended by 1000 students.

To the end, Teller had remarkable powers of concentration as illustrated by the following anecdote: in 1997, one of us (SBL) went to talk to Teller about a topic of mutual interest: numerical experimentation in mathematics, particularly number theory. As a preliminary, we were to discuss a compressed proof of Fermat's 'four square' theorem, which was written up (by SBL), along with some notes about related topics such as 'Gaussian sums.' However, this time, it wasn't possible to work at the board because he was blind. So he said, "read your notes, SLOOOWLY." Part way through, though unable to see, he took over the argument with a smile and completed the proof himself, messy algebra and all.

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# situations with energy densities above ordinary condensed matter beginning at about a kilojoule/cc or 10 kilobars.

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### Appendix:

Sidebars on the Jahn Teller effect and Gamow-Teller transitions

#### Jahn-Teller effect:

In general, corrections to the Born-Oppenheimer approximation arise from essentially linear 'vibronic' couplings linking the electronic states to the nuclear motion. If the electronic states are well separated in comparison to the matrix elements of the vibronic coupling, the corrections are perturbative. The Jahn-Teller effect arises in the opposite extreme: when the electronic terms are degenerate. Then, the molecule deforms in a non-perturbative way causing the terms to be concomitantly split, resulting in a unique ground state.

Taking a point example, consider consequences of differing valence for the Cu in the  $CuO_6$  octahedral complex within the  $K_2NiF_4$  type unit cell of the undoped perovskite high Tc superconductor precursor  $La_2CuO_4$  (see the figure below from Bednorz-Muller Nobel Prize lecture). As Bednorz and Muller point out, the possible configurations and terms for electrons in the  $CuO_6$  complex are built out of the assignment of the Cu d electrons to the appropriate representations of the cubic (octahedral) group. As usual in such a complex, the even parity (g) two dimensional representation orbitals  $e_{2g}$  originating from  $3z^2$ - $r^2$  and  $x^2$ - $y^2$  lie higher than the three dimensional representation orbitals  $t_{2g}$  arising from xy, yz, and zx. Thus, if the central copper ion is in a  $Cu^{3+}$  configuration ( $3d^8$ ), the higher  $e_{2g}$  orbitals are half filled. Therefore there is no orbital degeneracy and no deformation of the octahedral cell. But if the Cu is in a  $Cu^{2+}$  ( $3d^9$ ) configuration, the terms coming from  $e_{2g}$  are orbitally degenerate, with a resulting Jahn-Teller elongation of the octahedron.

#### Gamow-Teller transition:

Shortly after Fermi proposed his theory of beta decay (1934) in analogy with the matrix element for the electromagnetic interaction, Gamow and Teller argued for the necessity of a second type of matrix element: one that allowed for the decaying nucleus (or nucleon) to flip its spin. This observation arose in the context of the then rapidly developing knowledge of nuclear transitions and decays. If, as Fermi assumed, the matrix element entered at first order, the nuclear quantum numbers of the initial and final states carry the imprint of the interaction. Furthermore, the standard multipole expansion of the recoiling nucleus's wave function (e<sup>ipr</sup>) results in a sequence of increasingly forbidden transitions, each with appropriate selection rules (each power of pr giving a factor of about 1/100).

Focusing on the decay schemes of the 'thorium active deposit,' (see figure from the Gamow-Teller paper), Gamow and Teller noted that several of the natural spin assignments and beta and gamma decay rate rates in this scheme were in contradiction with the Fermi hypothesis. For example, because the spin of Th B ( $^{212}$ Pb<sub>82</sub>) is 0, it is impossible to interpret its rate of beta decay followed by quadrupole allowed gamma radiation into the ground state of Th C ( $^{212}$ Bi<sub>83</sub>) with the Fermi matrix element alone. This is because, in that theory, the decay would require two powers of pr to get J=2, causing the decay to be far too slow (assuming the phase space scales in the same way as a function of the emitted electron end point energy). However, with an additional matrix element of about the same strength allowing the nucleus to have j=1, this decay could be accommodated with a single power of pr.

In modern, relativistic notation, Gamow and Teller added a term to the Fermi beta decay Hamiltonian of the form:

$$\boldsymbol{H} = \sum C_A (\overline{\Psi_p} \gamma^\mu \gamma_5 \Psi_n) (\overline{\Psi_e} \gamma_\mu \gamma_5 \Psi_\nu) - C_T \frac{1}{4} (\overline{\Psi_p} [\gamma^\mu \gamma^\rho - \gamma^\rho \gamma^\mu] \Psi_n) (\overline{\Psi_e} [\gamma_\mu \gamma_\rho - \gamma_\rho \gamma_\mu] \Psi_\nu) + \boldsymbol{h.c.}$$

(where  $_{e}$  is a Dirac four-spinor for the emitted electron and g's are the standard gamma matrices and  $C_{F}$  (the Fermi coupling) and  $C_{GT} = (C_{A}C_{A}*+C_{T}C_{T}*)^{.5}$  are assumed to be of the same order of magnitude). In the non-relativistic limit, either of these possibilities  $(C_{A} \text{ or } C_{T})$  results in the same 'spin flip' possibility (later, of course,  $C_{T}$  was shown to be zero).

Interestingly, in the context of nuclear physics, the Gamow-Teller transition is much more common than the Fermi rule because of shell model effects. Of course, at the fundamental level (before 'renormalization') they are exactly the same strength as was first noticed in the leptonic sector, with important implications for the V-A theory and the subsequent development of electro-weak unification.

#### (figures courtesy of the AIP):

J. Georg Bednorz and K. Alex Muller, *Perovskite Type Oxides, the New Approach to High Tc Superconductivity*, Reviews of Modern Physics <u>60</u>, 585, (1988).

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